

# Jim Boelrijk | CV

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in jim-boelrijk

## Education

- 2020-Now **PhD AI4Science**, *Amsterdam Machine Learning Lab (AMLAB), Universiteit van Amsterdam*, Amsterdam, The Netherlands
- Supervisors: Bernd Ensing, Patrick Forré, Bob Pirok and Alfons Hoekstra
  - Topic of my PhD thesis:
    - Development of closed-loop optimization schemes using machine learning techniques.
    - Development of data-analysis techniques (peak detection, baseline correction, quantitative structure activity relationships) using machine learning techniques.
    - Equivariant/Invariant Deep learning frameworks.
- 2017-2019 **Master Chemistry (Track: Molecular Sciences, GPA: 8.5/10, cum laude)**, *Universiteit van Amsterdam*, Amsterdam, The Netherlands
- Title of my master's thesis:  
Incorporating maximally localized Wannier functions into neural network potentials
- 2015-2017 **Bachelor Chemistry**, *Universiteit van Amsterdam*, Amsterdam, The Netherlands
- 2012-2013 ○ Title of my bachelor's thesis:  
Vibrational Circular Dichroism of Glucose: Dynamic vs Static approaches
- 2006-2012 **Bilingual VWO, profile: Nature and Technology with extracurricular Economics**, *Hermann Wesselink college*, Amstelveen, The Netherlands

## Work Experience

- 2019-2020 **Software Tester**, *Software for Chemistry and Materials*, Netherlands
- Testing software changes in the AMS packages.
  - Testing software of competition from installment to benchmarks.
  - Creating general benchmark workflow in Python.
- 2013-2019 **Exam trainer**, *Lyceo*, Netherlands
- Preparing students for their high school exams in physics and chemistry.
  - Learned to explain things clearly.
- 2016-2016 **Temporary teacher**, *Inwijs*, Netherlands
- Temporarily replaced a chemistry and physics teacher. Taught chemistry and physics to 5th- and 6th-year VWO high school students.
  - Learned what it was like to plan lectures, explain matter to students and keep order.
- 2013-2015 **Professional Rugby Player**, *Stade Montois Rugby*, Mont-de-Marsan, France
- Was part of the youth academy (Under 23) of the professional rugby club Stade Montois.
  - Learned to work hard, be disciplined and to not give up easily.
  - Learned to adapt to a new environment and to the French language quickly.

## Selected Publications

- **Boelrijk, J.**, Pirok, B., Ensing, B., and Forré, P. Bayesian optimization of comprehensive two-dimensional liquid chromatography separations. *Journal of Chromatography A*, 2021
- **Boelrijk, J.**, van Herwerden D., Ensing B., Forré P, and Samanipour S. Predicting RP-LC retention indices of structurally unknown chemicals from mass spectrometry data. *ChemRxiv.*, 2022, submitted to Journal of Cheminformatics
- Bos, T, **Boelrijk, J.**, Molenaar, S, van 't Veer, B, Niezen, L, van Herwerden, D, Samanipour, S, Stoll, Dwight, Ensing B., Forré P, Somsen, G and B. Pirok. Chemometric Strategies for Fully Automated Interpretive Method Development in Liquid Chromatography *Analytical Chemistry*, 2022
- **Boelrijk, J.**, Ensing B., Forré P, and B. Pirok. Closed-loop automatic gradient design for liquid chromatography using Bayesian optimization. *Analytica Chimica Acta*, 2023
- **Boelrijk, J.**, Ensing B. and Forré P. Multi-objective optimization via equivariant deep hypervolume approximation. *ICLR 2023*

## Relevant Skills

### Programming

- Python
- Pytorch (including GPytorch and Botorch)
- Bash
- Matlab (limited)
- C++ (limited)

### Language proficiency

- Dutch (native)
- English (bilingual)
- French (professional)
- German (limited working)

## Awards and Achievements

- Youth player of the year 2012, best under 18 rugby player of the Netherlands
- Player for the National rugby team of the Netherlands (15 appearances so far).
- DELF B2 certificate in French.

## Miscellaneous

### Invited Talks

- AI4Science kickoff-workshop at the University of Amsterdam (09-07-2020)
- Illustere Alumni Event 2020 at the University of Amsterdam (19-11-2020)
- CHAINS KNCV Focus session on Machine learning for chemical discovery (07-12-2021)
- AMLAB Seminar at the University of Amsterdam (multiple)

### Teaching

- Teaching Assistant for Deep Learning 1 2021 (Master AI, University of Amsterdam)
- Teaching Assistant for Machine Learning 2 2020-2021 (Master AI, University of Amsterdam)
- Teaching Assistant for Machine Learning 1 2020 (Master AI, University of Amsterdam)
- Teaching Assistant for MolSim 2021, 2022 (Master Molecular Sciences / 2 week PhD Winter course)

### Organization

- Chair of the bi-weekly AI4Science Colloquium
- Maintenance of the AI4Science website

### Summer Schools

- Deep Learning + Reinforcement learning Summer School 2021 (DLRLSS 2021)